



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2026 – 10:42 AM EDT

PDB ID : 38XX / pdb_000038xx
Title : Crystal structure of a Formate acetyltransferase (PFL) from *Megasphaera* *lor-nae* with an acetylated active site cysteine
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2026-09-23
Resolution : 1.86 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

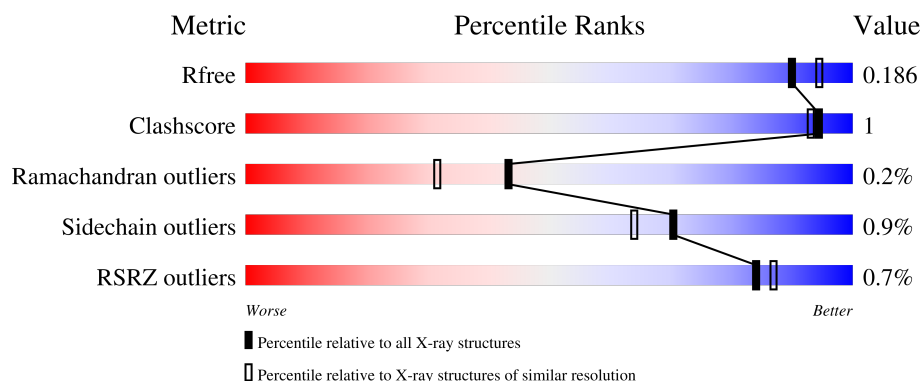
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	772	% 93%
1	B	772	% 94%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13272 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Formate acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	752	Total	C	N	O	S	0	8	0
			6081	3869	1027	1159	26			
1	B	752	Total	C	N	O	S	0	11	0
			6104	3882	1031	1165	26			

There are 42 discrepancies between the modelled and reference sequences:

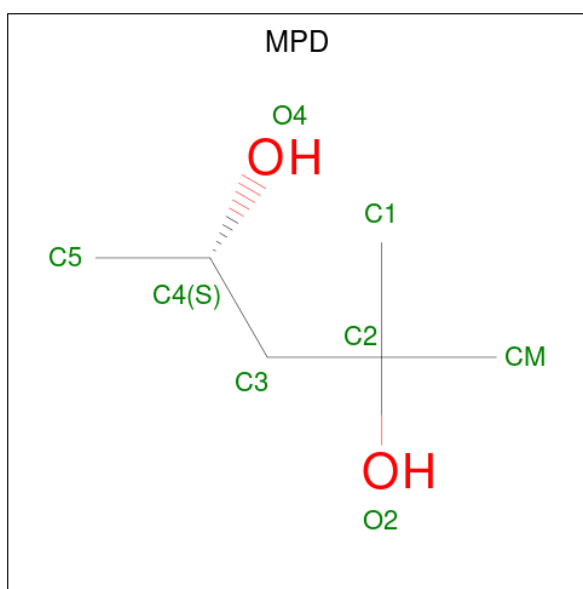
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0ABN0CZ30
A	-19	ALA	-	expression tag	UNP A0ABN0CZ30
A	-18	HIS	-	expression tag	UNP A0ABN0CZ30
A	-17	HIS	-	expression tag	UNP A0ABN0CZ30
A	-16	HIS	-	expression tag	UNP A0ABN0CZ30
A	-15	HIS	-	expression tag	UNP A0ABN0CZ30
A	-14	HIS	-	expression tag	UNP A0ABN0CZ30
A	-13	HIS	-	expression tag	UNP A0ABN0CZ30
A	-12	MET	-	expression tag	UNP A0ABN0CZ30
A	-11	GLY	-	expression tag	UNP A0ABN0CZ30
A	-10	THR	-	expression tag	UNP A0ABN0CZ30
A	-9	LEU	-	expression tag	UNP A0ABN0CZ30
A	-8	GLU	-	expression tag	UNP A0ABN0CZ30
A	-7	ALA	-	expression tag	UNP A0ABN0CZ30
A	-6	GLN	-	expression tag	UNP A0ABN0CZ30
A	-5	THR	-	expression tag	UNP A0ABN0CZ30
A	-4	GLN	-	expression tag	UNP A0ABN0CZ30
A	-3	GLY	-	expression tag	UNP A0ABN0CZ30
A	-2	PRO	-	expression tag	UNP A0ABN0CZ30
A	-1	GLY	-	expression tag	UNP A0ABN0CZ30
A	0	SER	-	expression tag	UNP A0ABN0CZ30
B	-20	MET	-	initiating methionine	UNP A0ABN0CZ30
B	-19	ALA	-	expression tag	UNP A0ABN0CZ30
B	-18	HIS	-	expression tag	UNP A0ABN0CZ30
B	-17	HIS	-	expression tag	UNP A0ABN0CZ30

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP A0ABN0CZ30
B	-15	HIS	-	expression tag	UNP A0ABN0CZ30
B	-14	HIS	-	expression tag	UNP A0ABN0CZ30
B	-13	HIS	-	expression tag	UNP A0ABN0CZ30
B	-12	MET	-	expression tag	UNP A0ABN0CZ30
B	-11	GLY	-	expression tag	UNP A0ABN0CZ30
B	-10	THR	-	expression tag	UNP A0ABN0CZ30
B	-9	LEU	-	expression tag	UNP A0ABN0CZ30
B	-8	GLU	-	expression tag	UNP A0ABN0CZ30
B	-7	ALA	-	expression tag	UNP A0ABN0CZ30
B	-6	GLN	-	expression tag	UNP A0ABN0CZ30
B	-5	THR	-	expression tag	UNP A0ABN0CZ30
B	-4	GLN	-	expression tag	UNP A0ABN0CZ30
B	-3	GLY	-	expression tag	UNP A0ABN0CZ30
B	-2	PRO	-	expression tag	UNP A0ABN0CZ30
B	-1	GLY	-	expression tag	UNP A0ABN0CZ30
B	0	SER	-	expression tag	UNP A0ABN0CZ30

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



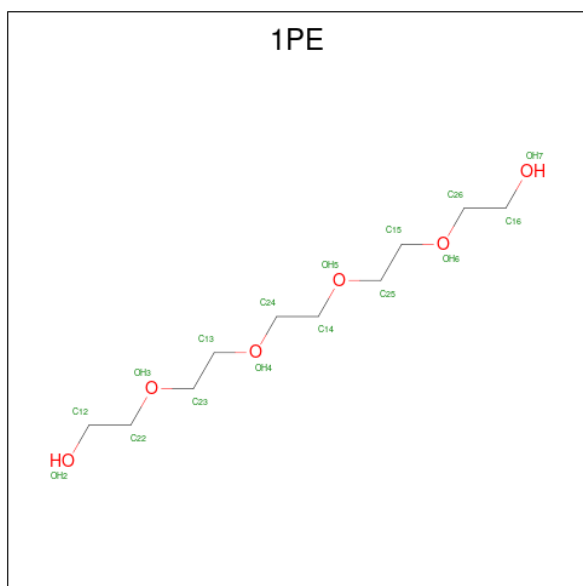
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		

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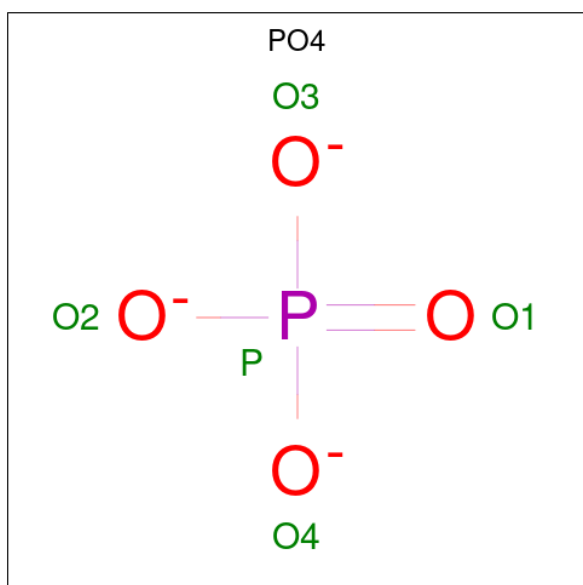
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

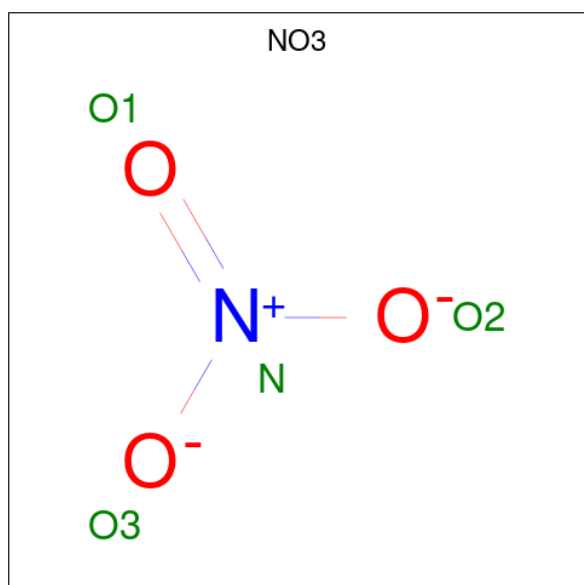


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

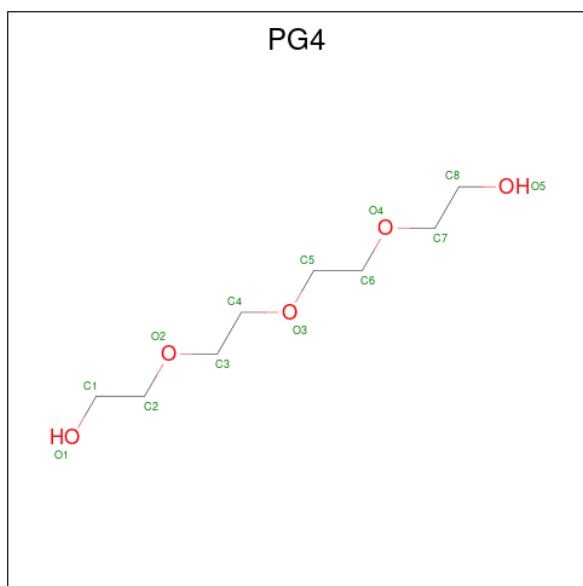
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0

- Molecule 6 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	N	O	0	0
			4	1	3		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			13	8	5		

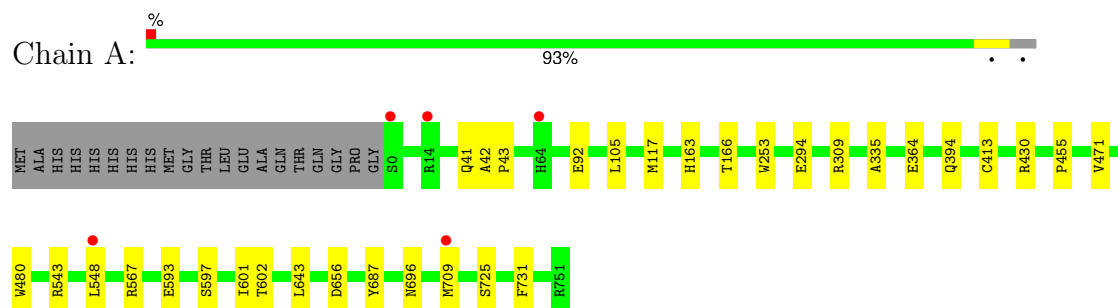
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	451	Total	O	0	0
			451	451		
8	B	529	Total	O	0	0
			529	529		

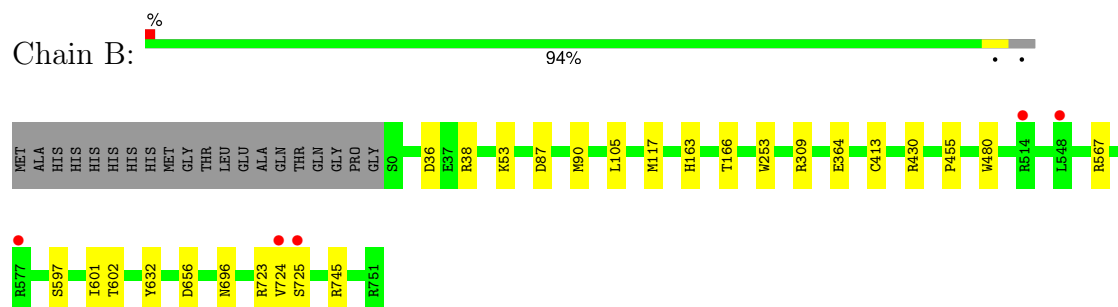
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Formate acetyltransferase



- Molecule 1: Formate acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.44Å 218.37Å 145.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 1.86 49.28 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.28-1.86) 99.9 (49.28-1.86)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 1.86Å)	Xtriage
Refinement program	PHENIX (2.0_5936: ???)	Depositor
R, R_{free}	0.157 , 0.179 0.165 , 0.186	Depositor DCC
R_{free} test set	7844 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.787	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.006 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13272	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0595e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, CL, PG4, MPD, PO4, NO3, SCY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/6219	0.48	0/8413
1	B	0.30	0/6248	0.49	0/8452
All	All	0.29	0/12467	0.49	0/16865

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6081	0	5923	18	0
1	B	6104	0	5942	13	0
2	A	16	0	28	2	0
2	B	16	0	28	1	0
3	A	16	0	22	0	0
4	A	20	0	0	1	0
4	B	20	0	0	0	0
5	A	1	0	0	1	0
5	B	1	0	0	1	0
6	B	4	0	0	0	0
7	B	13	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	451	0	0	0	0
8	B	529	0	0	0	0
All	All	13272	0	11961	31	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:ARG:HH12	2:B:801:MPD:HM1	1.41	0.84
1:A:567:ARG:HH12	2:A:802:MPD:HM1	1.47	0.78
1:A:471:VAL:HG13	2:A:801:MPD:HM3	1.85	0.58
1:B:87:ASP:OD2	1:B:90:MET:HE2	2.05	0.57
1:A:413:SCY:CD	5:A:808:CL:CL	2.94	0.52
1:B:413:SCY:CD	5:B:809:CL:CL	2.95	0.52
1:A:163:HIS:HA	1:A:166:THR:OG1	2.09	0.51
1:A:455:PRO:HD3	1:A:480:TRP:CE2	2.45	0.51
1:B:105:LEU:HD12	1:B:105:LEU:N	2.27	0.49
1:B:53:LYS:HE3	1:B:90:MET:CE	2.42	0.49
1:B:163:HIS:HA	1:B:166:THR:OG1	2.13	0.49
1:B:36:ASP:OD2	1:B:38[A]:ARG:HD3	2.16	0.46
1:B:597:SER:HB3	1:B:656:ASP:HB3	1.98	0.46
1:A:41:GLN:HG2	1:A:294:GLU:HG3	1.98	0.45
1:B:455:PRO:HD3	1:B:480:TRP:CD2	2.51	0.45
1:A:455:PRO:HD3	1:A:480:TRP:CD2	2.52	0.45
1:A:597:SER:HB3	1:A:656:ASP:HB3	1.99	0.45
1:A:394:GLN:HB3	1:A:696:ASN:OD1	2.16	0.45
1:A:41:GLN:CG	1:A:294:GLU:HG3	2.48	0.44
1:B:455:PRO:HD3	1:B:480:TRP:CE2	2.52	0.44
1:B:696:ASN:OD1	1:B:723[B]:ARG:NE	2.46	0.42
1:A:309:ARG:HG2	1:A:364:GLU:O	2.19	0.42
1:B:632:TYR:CE1	1:B:745:ARG:HG2	2.56	0.41
1:B:309:ARG:HG2	1:B:364:GLU:O	2.20	0.41
1:A:643:LEU:HB3	1:A:687:TYR:CD1	2.55	0.41
1:A:593:GLU:OE1	4:A:807:PO4:O2	2.39	0.41
1:A:709:MET:HG3	1:A:731:PHE:HE2	1.86	0.41
1:A:92:GLU:H	1:A:92:GLU:CD	2.28	0.41
1:A:543:ARG:HA	1:A:548:LEU:O	2.21	0.40
1:A:42:ALA:HB1	1:A:43:PRO:HD2	2.02	0.40
1:A:105:LEU:N	1:A:105:LEU:HD12	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	757/772 (98%)	733 (97%)	22 (3%)	2 (0%)	36	25
1	B	760/772 (98%)	735 (97%)	24 (3%)	1 (0%)	48	35
All	All	1517/1544 (98%)	1468 (97%)	46 (3%)	3 (0%)	43	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	601	ILE
1	B	601	ILE
1	A	335	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	635/646 (98%)	629 (99%)	6 (1%)	70	64
1	B	638/646 (99%)	630 (99%)	8 (1%)	61	51
All	All	1273/1292 (98%)	1259 (99%)	14 (1%)	70	57

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	MET
1	A	253	TRP
1	A	430	ARG
1	A	602	THR
1	A	725[A]	SER
1	A	725[B]	SER
1	B	117	MET
1	B	253	TRP
1	B	430	ARG
1	B	602	THR
1	B	724[A]	VAL
1	B	724[B]	VAL
1	B	725[A]	SER
1	B	725[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	161	HIS
1	A	191	GLN
1	A	228	GLN
1	A	719	ASN
1	B	28	ASN
1	B	228	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SCY	B	413	1	7,8,9	0.72	0	4,9,11	1.18	0
1	SCY	A	413	1	7,8,9	0.67	0	4,9,11	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SCY	B	413	1	-	1/5/7/9	-
1	SCY	A	413	1	-	1/5/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	413	SCY	CA-CB-SG-CD
1	B	413	SCY	CA-CB-SG-CD

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	413	SCY	1	0
1	A	413	SCY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	A	804	-	4,4,4	1.71	1 (25%)	6,6,6	0.40	0
4	PO4	B	807	-	4,4,4	1.68	1 (25%)	6,6,6	0.60	0
4	PO4	B	806	-	4,4,4	1.68	1 (25%)	6,6,6	0.67	0
6	NO3	B	803	-	1,3,3	0.14	0	0,3,3	-	-
4	PO4	A	806	-	4,4,4	1.66	1 (25%)	6,6,6	0.56	0
7	PG4	B	804	-	12,12,12	0.28	0	11,11,11	0.21	0
2	MPD	A	801	-	7,7,7	0.45	0	9,10,10	0.54	0
4	PO4	B	808	-	4,4,4	1.64	1 (25%)	6,6,6	0.57	0
4	PO4	A	807	-	4,4,4	1.55	1 (25%)	6,6,6	0.55	0
4	PO4	B	805	-	4,4,4	1.54	1 (25%)	6,6,6	0.69	0
2	MPD	B	802	-	7,7,7	0.35	0	9,10,10	0.76	0
2	MPD	B	801	-	7,7,7	0.29	0	9,10,10	0.71	0
3	1PE	A	803	-	15,15,15	0.31	0	14,14,14	0.32	0
2	MPD	A	802	-	7,7,7	0.35	0	9,10,10	0.62	0
4	PO4	A	805	-	4,4,4	1.86	1 (25%)	6,6,6	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PG4	B	804	-	-	1/10/10/10	-
2	MPD	A	801	-	-	1/5/5/5	-
2	MPD	B	802	-	-	0/5/5/5	-
2	MPD	B	801	-	-	1/5/5/5	-
3	1PE	A	803	-	-	5/13/13/13	-
2	MPD	A	802	-	-	1/5/5/5	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	805	PO4	P-O1	3.25	1.58	1.50
4	A	804	PO4	P-O1	2.90	1.57	1.50
4	B	806	PO4	P-O1	2.86	1.57	1.50
4	B	808	PO4	P-O1	2.84	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	807	PO4	P-O1	2.82	1.57	1.50
4	A	806	PO4	P-O1	2.78	1.57	1.50
4	A	807	PO4	P-O1	2.68	1.56	1.50
4	B	805	PO4	P-O1	2.56	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	1PE	OH2-C12-C22-OH3
3	A	803	1PE	OH6-C15-C25-OH5
7	B	804	PG4	O1-C1-C2-O2
3	A	803	1PE	C23-C13-OH4-C24
2	A	802	MPD	O2-C2-C3-C4
2	B	801	MPD	O2-C2-C3-C4
3	A	803	1PE	C15-C25-OH5-C14
3	A	803	1PE	OH5-C14-C24-OH4
2	A	801	MPD	CM-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	MPD	1	0
4	A	807	PO4	1	0
2	B	801	MPD	1	0
2	A	802	MPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	751/772 (97%)	-0.02	5 (0%) 84 87	18, 37, 58, 90	8 (1%)
1	B	751/772 (97%)	-0.11	5 (0%) 84 87	17, 34, 51, 85	11 (1%)
All	All	1502/1544 (97%)	-0.06	10 (0%) 84 87	17, 35, 56, 90	19 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	724[A]	VAL	4.2
1	A	0	SER	2.6
1	B	548	LEU	2.5
1	A	64	HIS	2.2
1	B	514	ARG	2.2
1	A	709	MET	2.1
1	B	725[A]	SER	2.1
1	A	548	LEU	2.1
1	B	577	ARG	2.1
1	A	14	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SCY	B	413	9/10	0.95	0.09	27,28,31,33	0
1	SCY	A	413	9/10	0.97	0.09	31,33,35,36	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PO4	B	807	5/5	0.50	0.14	72,73,85,88	0
6	NO3	B	803	4/4	0.66	0.13	51,52,53,56	0
3	1PE	A	803	16/16	0.70	0.18	59,65,71,71	0
4	PO4	A	805	5/5	0.70	0.13	53,56,72,79	0
4	PO4	A	804	5/5	0.75	0.17	43,45,50,53	5
2	MPD	A	802	8/8	0.75	0.17	54,57,57,60	0
7	PG4	B	804	13/13	0.77	0.15	54,58,63,64	0
4	PO4	B	806	5/5	0.79	0.12	54,54,69,82	0
4	PO4	A	806	5/5	0.79	0.10	60,63,74,82	0
4	PO4	B	808	5/5	0.80	0.15	54,56,70,74	0
4	PO4	A	807	5/5	0.85	0.13	57,59,72,74	0
2	MPD	B	801	8/8	0.85	0.14	48,51,55,56	0
2	MPD	A	801	8/8	0.87	0.16	49,53,54,57	0
4	PO4	B	805	5/5	0.89	0.17	35,35,38,39	5
2	MPD	B	802	8/8	0.92	0.12	44,45,49,51	0
5	CL	B	809	1/1	0.95	0.10	40,40,40,40	0
5	CL	A	808	1/1	0.97	0.12	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.